

Incorporating Uncertainties in Satellite-Derived Chlorophyll into Model Forecasts

Gould, R.W., Jr.¹, S.C. McCarthy¹, E. Coelho², I. Shulman¹, S. Anderson¹, and P. Sakalauskas¹

¹Code 7331, Naval Research Laboratory, Stennis Space Center, MS, USA 39529

²Department of Physics, University of New Orleans, Stennis Space Center, MS, USA 39529

ABSTRACT

We describe and apply an ensemble approach, similar to that used in environmental modeling, to quantify errors and produce uncertainty maps for satellite-derived ocean color chlorophyll, and we incorporate these uncertainties into hydrodynamic and biophysical models. Ensemble techniques allow the propagation and assessment of error sources, including those due to sensor calibration, sensor drift, atmospheric correction, and bio-optical inversion algorithms, through the end-to-end image processing stream. For an ocean color image, we first apply realistic noise to the satellite top-of-atmosphere radiances, which leads to an ensemble of chlorophyll values at each image pixel (and thus an ensemble of chlorophyll images). From this ensemble, we derive mean and standard deviation (uncertainty) images for the chlorophyll, which we then incorporate into both hydrodynamic and biophysical forecast models. The image of chlorophyll uncertainty allows improved estimates of correlation scales and error covariances in the models. There are two approaches to produce short-term (1-3 day) forecasts of bio-optical properties: (1) treat the property as a conservative tracer and advect a satellite-observed distribution forward in time using current fields from a hydrodynamic model, and (2) use a fully-coupled biophysical process model that includes applicable sources and sinks. The first case does not include biology in the simulation (it only accounts for dynamical processes such as winds, currents, and tides), whereas the second case does. For both these cases, we create forecast ensemble suites, where each ensemble member uses a different realization (e.g., forcing and/or initial field); the ensemble spread (variance) provides an indication of uncertainty, or confidence in the chlorophyll forecast. We examine mean and individual forecast ensemble members (R^2 , spread-skill statistics) to assess predictive value. Thus, we produce a final chlorophyll forecast field that includes uncertainties in both the initial satellite chlorophyll values as well as uncertainties in the hydrodynamic and biological models.

INTRODUCTION

Typically, to address uncertainties in satellite-retrieved water reflectances and bio-optical properties, the satellite values are compared to in situ measurements (Antoine et al., 2008), but this approach has limitations. Due to cloud cover in the satellite imagery, and the expense and spatial/temporal coverage limitations associated with in situ data collection, there are often very few match-ups between the satellite and in situ values, particularly for regional comparisons. With regard to satellite ocean color image products, such as the chlorophyll concentration, they are typically provided without any indication of the uncertainty in the estimation, so the end-user (scientists, coastal managers, and military personnel) have very limited information on the reliability of the satellite retrievals for a specific image.

To help address this shortcoming, we have extended an approach used by the numerical modeling community to satellite ocean color imagery. In environmental modeling, for example in the physical and meteorological communities, ensembles are generated to assess model errors and improve

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hydrodynamic and weather forecasts. The “spaghetti plots” of potential hurricane tracks are a familiar example. Monte-Carlo methods are applied to perturb the dominant sources of uncertainties (e.g. initial and boundary conditions, model physics, atmospheric forcing, etc.) in the forecast model. An ensemble forecast suite is generated; the ensemble mean represents the “best-guess” forecast track, and the ensemble variance or standard deviation represents a proxy estimate for the uncertainty in the forecast. Statistics and metrics can be utilized (ensemble mean, RMS error, and spread) to provide some estimate of how well the ensembles capture “reality,” thereby providing insight into the underlying deterministic processes and aiding decision support.

There are multiple error sources throughout the processing of satellite ocean color imagery. At each step of the processing, from measurement of top-of-the-atmosphere (TOA) radiances, through atmospheric correction, bio-optical inversion, and bio-optical forecasting, uncertainties propagate and are intertwined. Thus, ocean color image processing should lend itself to an ensemble approach to address the error cascading through the various steps; we have developed such an approach to partition and assess the error sources. We apply an ensemble of random noise (each ensemble applies $\pm 2\%$ random noise across an image) to the TOA radiance values. To partition the error sources, we apply the noise to separate sets of wavebands. For example, to examine the effect of noise (sensor radiance measurement uncertainty) during the atmospheric correction process, we apply noise only to the TOA radiances in the two near-infrared (NIR) MODIS channels used in the atmospheric correction routines (748 and 869 nm bands). To examine the effect of noise on the bio-optical inversion algorithms, we apply noise only to the TOA radiances in the seven visible MODIS channels used in the estimation of the bio-optical products, such as chlorophyll, absorption and backscattering coefficients (412, 443, 488, 531, 547, 667, 678 nm bands). The Figure 1 schematic summarizes the ensemble approach applied to satellite ocean color imagery.

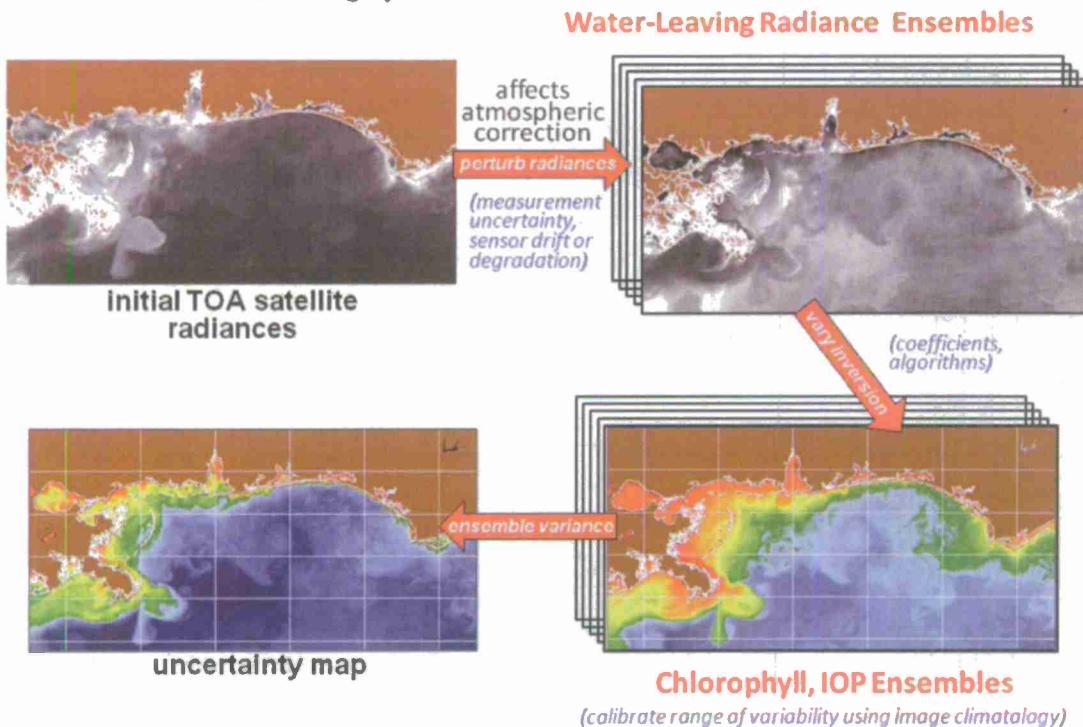


Figure 1. Schematic representation of the ensemble process applied to satellite ocean color imagery. The goal is to derive an uncertainty estimate for the bio-optical products (chlorophyll in this example), using the ensemble variance as a proxy.

In addition, we are interested in forecasting the bio-optical products (in this case, chlorophyll) by coupling the satellite images with hydrodynamic and biological models. We would like to propagate the uncertainties in the chlorophyll image values through the modeling process. There are two approaches to produce short-term (1-3 day) forecasts of bio-optical properties: Case (1) treat the property as a conservative tracer and advect a satellite-observed distribution forward in time using current fields from a hydrodynamic model, and case (2) use a fully-coupled biophysical process model that includes applicable sources and sinks. The first case does not include biology in the simulation (it only accounts for dynamical processes such as winds, currents, and tides), whereas the second case does. We examine both of these cases. Initially, for the first case, we forecast the chlorophyll distribution without any uncertainty in the initial image, and we compare this with the modeling result including uncertainty (from the chlorophyll ensembles). Since the second case relies on the biological model spin-up to equilibrium to set initial chlorophyll distributions (rather than a satellite chlorophyll field), the satellite chlorophyll uncertainties are not included for this case. Although not presented here, we will use the satellite uncertainties to improve the spatial representation of the chlorophyll error covariances in the model. Ultimately, we will assimilate satellite bio-optical products into the coupled bio-physical model; some of that work will be presented by Shulman et al. (2012) at this conference. Figure 2 shows the conceptual framework.

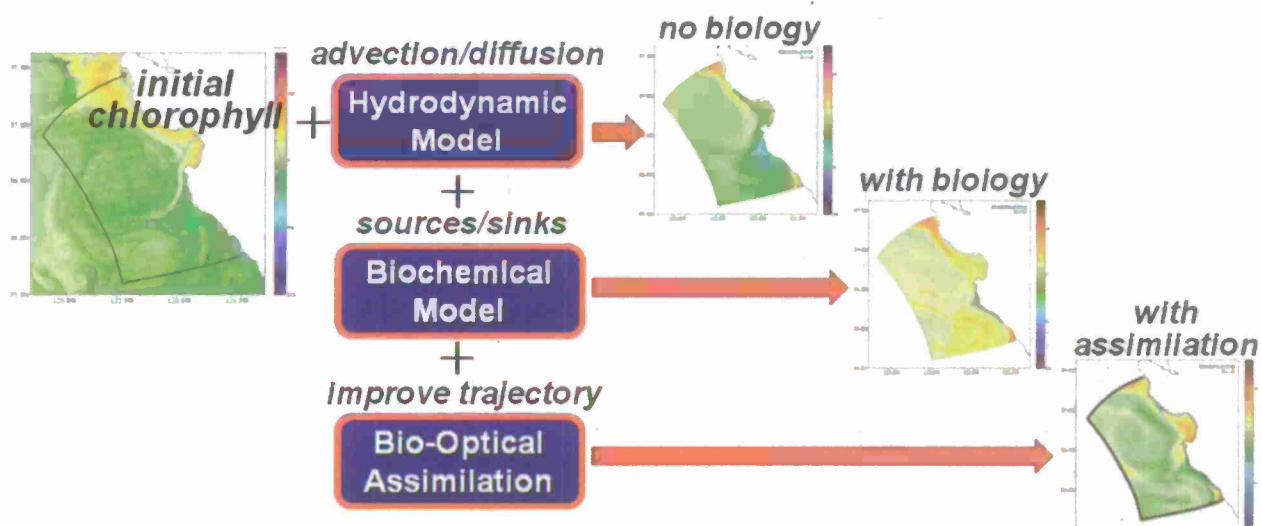


Figure 2. Schematic representation of the modeling framework for bio-optical forecasting. Progression from advection of chlorophyll as a passive tracer using a hydrodynamic model, to incorporation of source/sink terms with a coupled biochemical model, to ultimate assimilation of satellite ocean color imagery.

OBJECTIVES

Our objectives are to: (1) apply noise to satellite TOA radiances in an ensemble approach to quantify uncertainties in satellite-derived ocean color chlorophyll estimates; (2) determine whether the ensembles are realistic; (3) generate ensembles using different wavelength sets to partition the uncertainties at various stages of the processing (atmospheric correction, bio-optical inversion) to assess the effect of the uncertainties on the chlorophyll images; (4) incorporate the uncertainties into hydrodynamic and biophysical model simulations; (5) assess the effect of biology in the simulations and the impact of the chlorophyll uncertainties on the model forecast fields.

METHODS

The Naval Research Laboratory (NRL) at the Stennis Space Center (SSC) in Mississippi has developed an Automated Processing System (APS) that ingests and processes AVHRR, SeaWiFS, MODIS, MERIS, and OCM satellite imagery (Martinolich and Scardino, 2011). APS is a powerful, extendable, image-processing tool. It is a complete end-to-end system that includes sensor calibration, atmospheric correction (with near-infrared correction for coastal waters), image de-striping, and bio-optical inversion. APS incorporates the latest NASA MODIS code and enables us to produce the NASA standard SeaWiFS and MODIS products, as well as Navy-specific products using NRL algorithms. We can reprocess many data files (dozens of scenes/day). We maintain compatibility with NASA/Goddard algorithms and processing code. All imagery was processed with consistent atmospheric correction and bio-optical algorithms using the NRL APS version 4.6, which is consistent with SeaDAS version 6.3. An iterative, near-infrared atmospheric correction tuned for coastal waters was applied (Stumpf et al., 2003).

Satellite Imagery/Processing

With the NRL APS, the architecture is in place for the image ensemble analysis. From an initial MODIS image, we simply create an ensemble of new images by applying the $\pm 2\%$ random noise to the TOA radiance values. Each ensemble image is then reprocessed through APS to yield an ensemble of derived products, such as normalized water-leaving radiances (nLw) and chlorophyll (that we examine here) among others. The random noise that is applied to the TOA radiances varies spectrally, but is held constant across an image. For the analyses below, we produce either 100 image ensembles (for the error partitioning analyses) or 20 image ensembles (for the hydrodynamic advection forecast). To assess the reality or “representativeness” of the generated ensemble suite, we compare the variability in the ensemble results to the natural variability observed in a 2-year climatology of imagery covering the same region (2006-2007 northern Gulf of Mexico).

Hydrodynamic Model

To advect the surface SeaWiFS satellite chlorophyll field and produce 24, 48, and 72-hour forecast simulations, we used currents derived from the Relocatable Navy Coastal Ocean Model (RELO-NCOM). RELO-NCOM is based on a standardized development and an efficient configuration management to facilitate transitions of new tools and real-time configurations of regional high resolution (order 1 km) ocean predictions. The physics and numerical procedures of NCOM are based on the Princeton Ocean Model (POM) and a Sigma/Z-level Model (SZM). It is a primitive-equation, 3D, hydrostatic model that solves a three-dimensional, primitive equation, baroclinic, hydrostatic and free surface system using a cartesian horizontal grid, a combination of σ/z level (i.e., bottom-following/constant depth) vertical grid and implicit treatment of the free surface (Ko et al., 2008). It uses the Mellor-Yamada level 2.5 turbulence closure scheme, and the Smagorinsky formulation for horizontal mixing (Martin 2000). For mesoscale real-time applications, boundary conditions are taken from an operational run of the global NCOM (GNCOM). The domain of this particular experiment covered the entire Gulf of Mexico (18N 98W, 40N 79W), from 1 April to 30 October 2010. The atmospheric forcing was taken from the regional 15km COAMPS run by the Fleet Numerical Meteorological and Oceanographic Center (FNMOC). Tides were introduced at the boundaries and through local tidal potentials. The horizontal grid spacing was set at 3km and used 50 sigma/z levels in the vertical. The model assimilates local in-situ observations along with satellite altimetry and sea-surface temperature (SST) data using a combination of model analysis and data; all available observations from global and local data bases were assimilated over the full period.

For the chlorophyll forecasts with the hydrodynamic model (Case 1 in the INTRODUCTION), a “pseudo 3-dimensional” Eulerian advection scheme was used (without molecular or turbulent diffusion terms). With this approach, there are essentially two vertical layers, a 1 meter-thick surface layer and a conceptual deep layer to preserve continuity (i.e., there is vertical flux between the two layers, but they move together horizontally). These simulations only include current advection and an assumed uniform vertical chlorophyll distribution based on the surface values. Future enhancements will include addition of diffusion terms, full 3D vertical layering, and the capability to include more realistic vertical chlorophyll profiles. The forecast simulations do not include any assimilation of in situ chlorophyll data or additional satellite imagery, so currently the values are unconstrained. Also, with this approach, there is an implicit assumption that the bio-optical property (chlorophyll) is conservative. Although this is not strictly true, of course, it may be approximately valid over the short time scales (1-3 days) that we are examining, particularly in coastal areas where transport processes might be expected to dominate biological processes. Therefore, we consider the optical properties to be “pseudo-conservative” tracers for our purposes. This allows us to ignore growth and grazing terms for this case and treat the distributional changes as though they are due entirely to dynamical processes (Gould et al., 2008).

Coupled Biophysical Model

For the chlorophyll forecasts with the coupled hydrodynamic and ecological model (Case 2 in the INTRODUCTION), we couple NCOM with the Carbon, Silicon, Nitrogen Ecosystem (CoSINE) model (Chai et al., 2002), and perform simulations in Monterey Bay, California. In this case, source/sink terms (growth, grazing) are explicitly modeled, so chlorophyll is no longer considered a passive tracer as in Case 1. We examine model runs with and without biology included, to examine the differences in the forecast results.

The Monterey Bay model consists of the physical model (Shulman et al., 2007), which is coupled to the biochemical model (Chai et al., 2002, Shulman et al., 2011). The physical model of the Monterey Bay is based on the NCOM model described above. The Monterey Bay model is set up on a curvilinear orthogonal grid with resolution ranging from 1 to 4 km. The model is forced with surface fluxes from the Coupled Ocean and Atmospheric Mesoscale Prediction System (COAMPS) (Doyle et al., 2009) at 3 km horizontal resolution. The 3-km resolution COAMPS grid mesh is centered over Central California and the Monterey Bay. The biochemical model (CoSINE) of the Monterey model simulates dynamics of two sizes of phytoplankton, small phytoplankton cells ($< 5 \mu\text{m}$ in diameter) and diatoms, two zooplankton grazers, nitrate, silicate, ammonium, and two detritus pools. Phytoplankton photosynthesis in the biochemical model is driven by Photosynthetically Active Radiation (PAR), which is estimated based on the shortwave radiation flux from the COAMPS model. The Penta et al. (2008) scheme is used for PAR attenuation with depth. Open boundary conditions for the Monterey Bay model are derived from the regional model of the California Current (NCOM CCS, Shulman et al., 2007). The NCOM CCS has a horizontal resolution of about 9 km and, the model is forced with atmospheric products derived from the COAMPS (Doyle et al., 2009). As in NCOM ICON model, the biochemical model of the NCOM CCS is also 9-compartment model of Chai et al. (2002).

RESULTS

As an example test case, we selected the MODIS 14 October 2011 image covering the northern Gulf of Mexico for ensemble analysis. As mentioned above, we generated 100 chlorophyll ensembles from this image by randomly applying $\pm 2\%$ noise to the TOA radiances in the visible and NIR bands.

Different random noise was applied to each band, but there was no variation from pixel-to-pixel (i.e., it was constant across the scene). Figure 3 shows the mean chlorophyll image from the ensemble suite and the associated uncertainty image (the ensemble standard deviation).

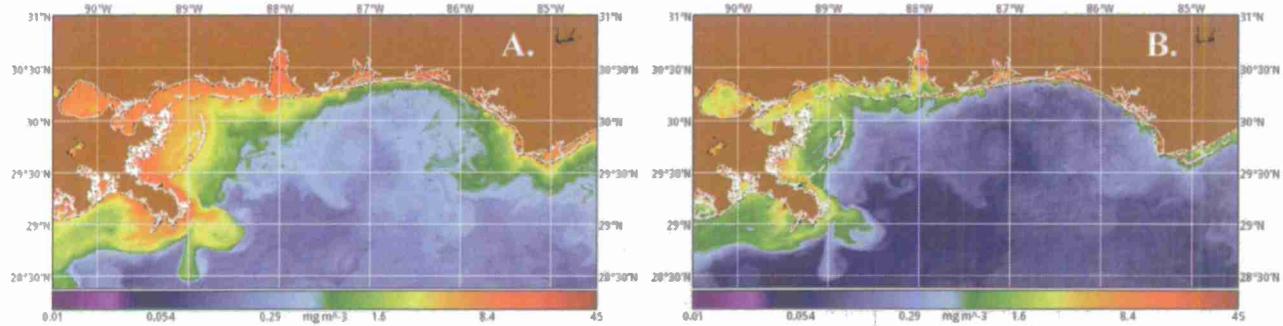


Figure 3. MODIS 14 October 2011. A. Mean ensemble chlorophyll. B. Ensemble chlorophyll standard deviation (proxy for uncertainty).

An initial step with the use of ensembles is to assess whether the ensemble suite adequately represent reality. In other words, is the ensemble variability representative of natural variability? For this assessment, since we applied noise to the image TOA radiances (L_t), we compared the ensemble L_t radiances to the L_t radiances from the original image, and to mean L_t radiances derived from selected clear MODIS scenes covering the same area over a 2-year period from 2006-2007 (Figure 4). We refer to the 2-year values as climatological values. The values in Figure 4 are spatial averages across the entire scene, as well as temporal averages over the 2-year period. The ensemble mean and original L_t values, and the minimum/maximum values are nearly identical (Figure 4a). Also, for the most part, the natural variability derived from the climatology encompasses the ensemble variability, although the mean values for this image (original as well as ensemble values) are lower than the climatological means at all wavelengths (Figure 4b).

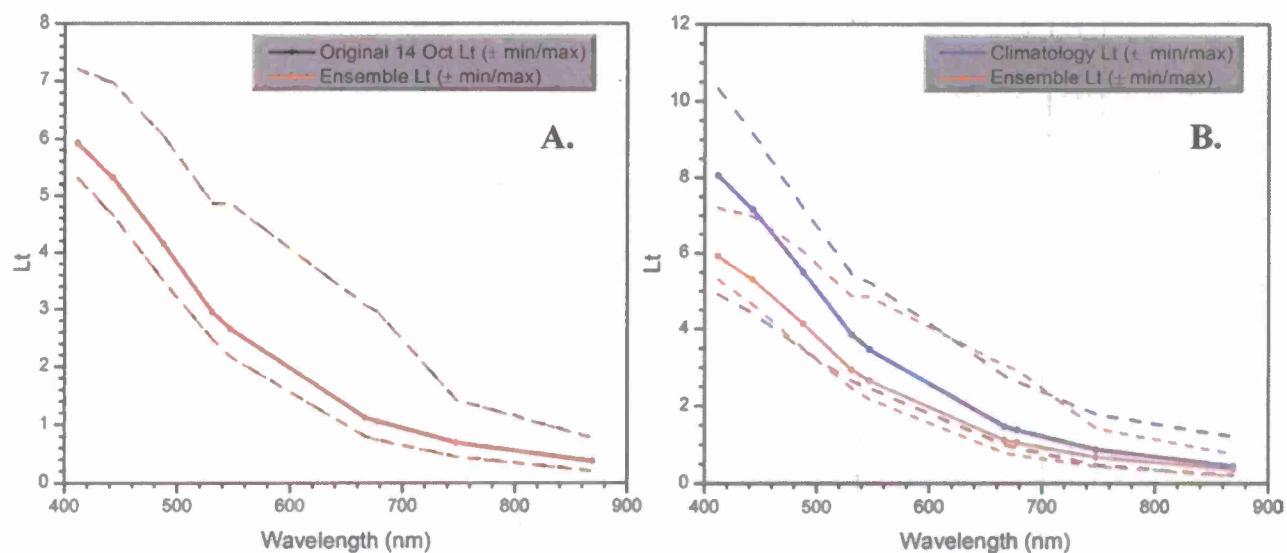


Figure 4. L_t radiance (mean, minimum/maximum values) vs. wavelength. A. Original 14 October 2011 radiances and ensemble radiances. B. Climatological radiances and ensemble radiances.

So, the ensemble suite is not generating “unusual” variability outside the realm of observed or natural variability, and our assessment is that the ensemble suite is realistic. Also, the vicarious gain coefficients that are applied to the MODIS Lt values during calibration are in the range of 2-3% (http://oceancolor.gsfc.nasa.gov/VALIDATION/operational_gains.html), similar to the noise ranges that we are applying here.

We also examined the effect of the Lt noise on the derived normalized water-leaving radiance (nLw) values, to verify that the radiance values following atmospheric correction were also realistic. Again, we compared the ensemble values to the original values and the climatological values (Figure 5). The ensemble nLw values at the short wavelengths are slightly higher than the original values (Figure 5A). Both the ensemble and original nLw values are significantly lower than the climatological values at 412 nm, but the mean and min/max values are generally similar at the other wavelengths (Figure 5B). As a result of the slightly higher nLw radiances for the ensemble mean as compared to the original values, the chlorophyll distribution is skewed to slightly lower values across the scene (Figure 6A). This is also apparent in the frequency distribution of the percent differences between the original chlorophyll values and the ensemble chlorophyll values (Figure 6B).

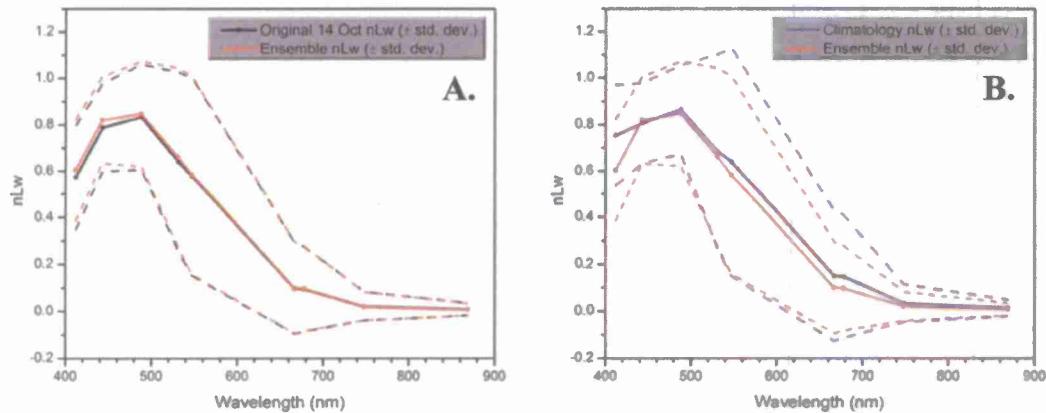


Figure 5. nLw radiance (mean, minimum/maximum values) vs. wavelength. **A.** Original 14 October 2011 radiances and ensemble radiances. **B.** Climatological radiances and ensemble radiances.

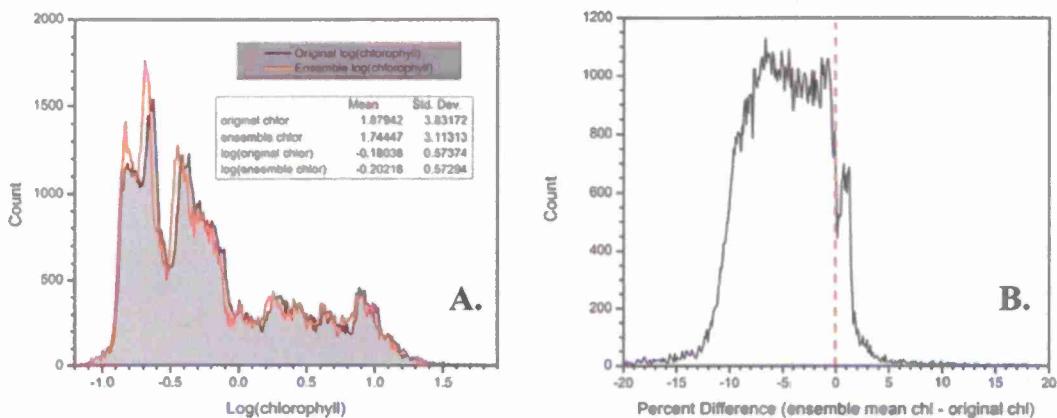


Figure 6. Chlorophyll frequency distributions, ensemble mean vs. original. **A.** Log chlorophyll values. **B.** Percent difference between ensemble mean and original chlorophyll values.

We also examined the spatial distributions of the differences between the mean ensemble and original chlorophyll values; Figure 7 shows the percent differences. We first apply noise to the Lt values in both the visible and NIR channels (Figure 7A). This demonstrates the noise impact on the complete processing. Then, by only applying noise to the Lt values in the two NIR bands (748, 869 nm), we can assess the effects of the noise due to only the atmospheric correction process (i.e., differences due to different aerosol selection models, Figure 7B). Similarly, by only applying noise to the visible channels (412, 443, 488, 531, 547, 667, 678 nm), we can assess the effects of the noise on the bio-optical inversion algorithms. Figure 7A indicates that the mean ensemble chlorophyll values are generally lower than the original chlorophyll values by about 5-10% when noise is applied to all channels (c.f. Figure 6B). A much lower percent difference is observed when noise is applied to just the NIR channels (Figure 7B). When noise is applied to just the visible wavelengths, some mean ensemble chlorophyll values are higher than the original values in certain parts of the image (yellow pixels in Figure 7C). Using this partitioning, we can also examine the separate effects on the uncertainty distributions (Figure 8). Figure 8A shows the coefficient of variation (expressed as the standard deviation percent of the mean) across the image, when Lt noise is applied to all wavelengths (both visible and NIR). Figure 8B shows the result when noise is applied only to the NIR bands, and Figure 8C shows the results for noise applied only to the seven visible bands. As in Figure 7, Figure 8 indicates that most of the uncertainty is associated with adding noise to the visible band, as opposed to adding noise to the NIR bands.

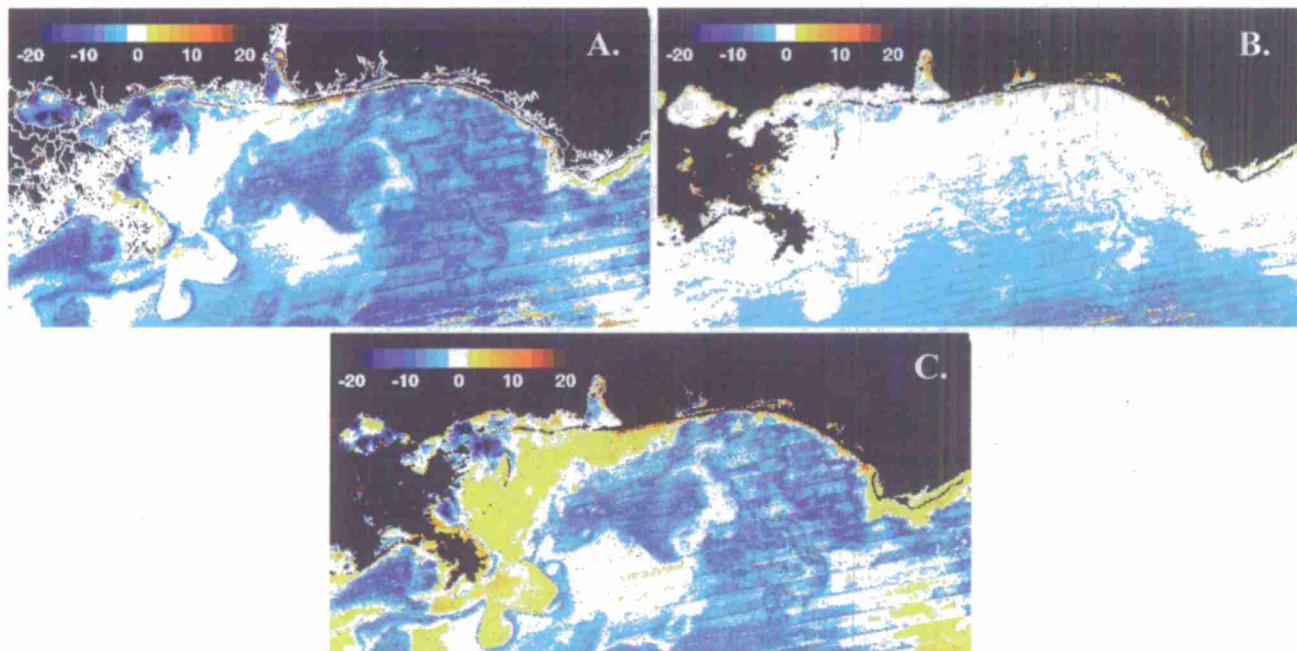


Figure 7. Percent difference between the ensemble mean chlorophyll and the original chlorophyll for the 14 October 2011 MODIS image. A. Lt noise applied to both NIR and visible wavelengths. B. Lt noise applied to just NIR wavelengths. C. Lt noise applied to only the visible wavelengths. Blue pixels indicate the original chlorophyll values were larger than the ensemble values, yellow pixels, vice versa.

Chlorophyll Forecasts - Hydrodynamic Model

To access and estimate uncertainty in chlorophyll forecasts using only a hydrodynamic model (treating chlorophyll as a passive tracer, Case 2 in the INTRODUCTION), we examined a clear, 3-day period

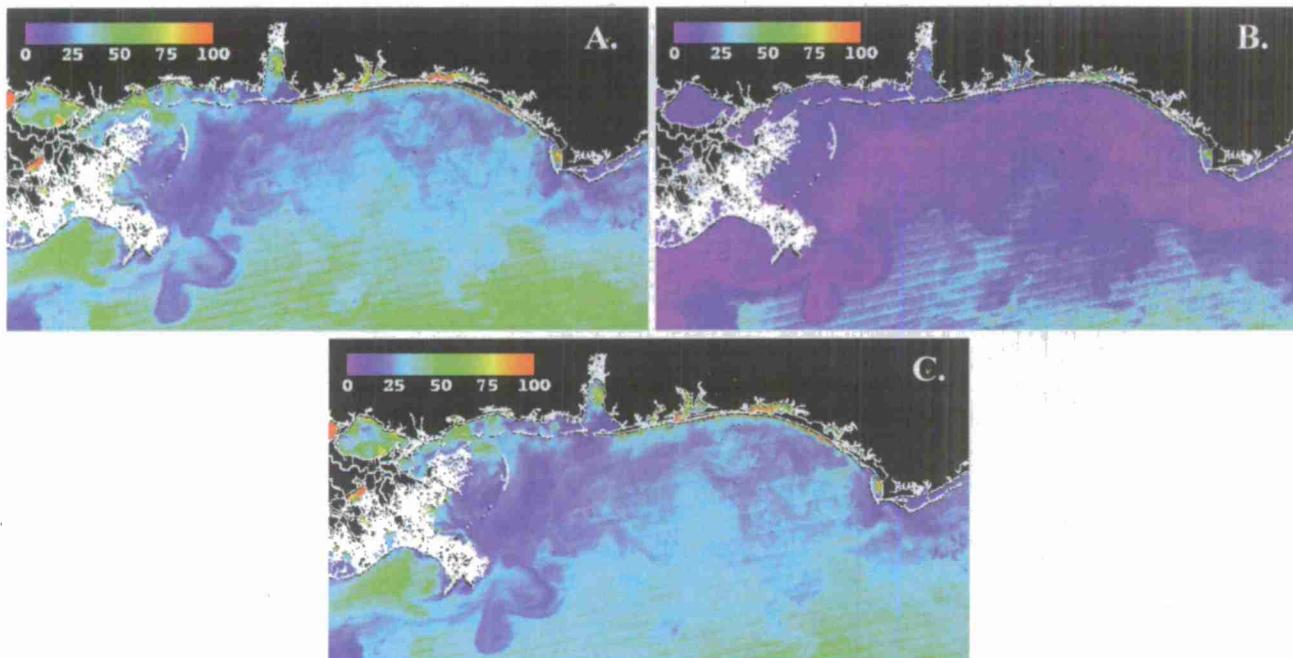


Figure 8. Chlorophyll standard deviation percent of mean (partitioned uncertainty) for the 14 October 2011 MODIS image. A. Lt noise applied to both NIR and visible wavelengths. B. Lt noise applied to just NIR wavelengths. C. Lt noise applied to only the visible wavelengths.

(14-17 October) covering the Mississippi Bight region in the northern Gulf of Mexico in 2011. This hydrodynamic approach only accounts for dynamical processes (winds, currents, tides) and does not include biogeochemical mechanistic processes (growth, grazing); it allowed us to examine the effect of only current variability on the bio-optical forecasts. An ensemble of 20 chlorophyll images was generated for the initial 14 October MODIS scene by applying random noise ($\pm 2\%$) to the Lt radiances for all the visible (7) and NIR (2) channels. An ensemble of 32 ocean model members was generated by varying initial and boundary conditions, and atmospheric forcing. Thus a total of 640 (32x20) chlorophyll forecasts were generated by advecting the initial chlorophyll image from 14 October (with noise included through the 20 ensembles) for three days with the 32 ocean ensembles. In Figure 9A, the mean ensemble chlorophyll forecast resulting from this simulation is shown for 17 October, along with the MODIS image for the same day for comparison (Figure 9B). A spread-skill scatter plot of the standard deviation of the observed mismatch between the forecast and observed distribution vs. the ensemble predicted standard deviation is shown in Figure 9C. Good spread-skill (a linear distribution following the one-to-one line) indicates that the predicted variance increases with the mismatch variance. In the example shown here, the ensemble predicted standard deviation values are slightly higher than the observed mismatch standard deviations for the low values, but, in general, the forecast demonstrates good spread-skill with both properties increasing fairly linearly.

Chlorophyll Forecasts - Coupled Biophysical Model

To access and estimate uncertainty in chlorophyll forecasts using a coupled bio-physical model (Case 2 in the INTRODUCTION), we have created two ensembles of the Monterey Bay model runs. Ensemble 1 (E1) consists of 10 coupled bio-chemical, physical model runs for the Monterey Bay area (Shulman et al., 2011). Two factors affecting the bio-chemical, physical model variability were considered: the amount of physical observations assimilated and the choices of the vertical coordinate system in the model. For each model run in the E1 ensemble, the chlorophyll was derived from the constituents of

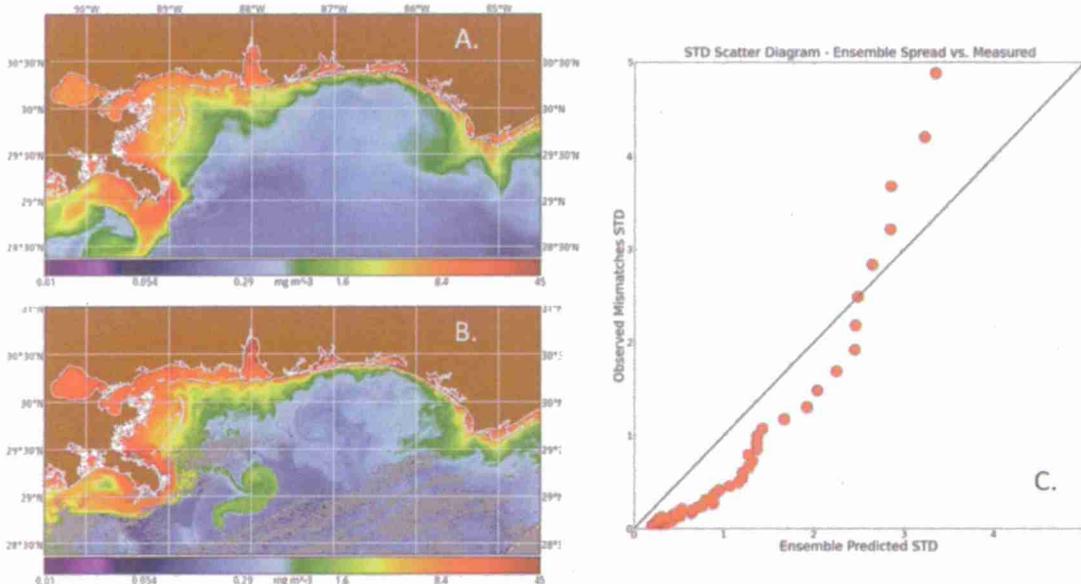


Figure 9. A. Forecast ensemble mean chlorophyll for 17 October 2011 (3-day simulation). B. MODIS image for 17 October 2011. C. Spread-skill metric plot.

the bio-chemical model (CoSINE) coupled to the physical model (NCOM). Ensemble 2 (E2) consists of the same 10 model runs as E1, but the bio-chemical component of the coupled model was turned off. Instead, in each member of E2, the chlorophyll was treated as a passive tracer (controlled only by advective and diffusive processes of the physical model). Both ensembles (E1 and E2) were initialized on 19 April of 2008, and spun up until 2 June. On June 2, the second ensemble run (E2) was started with biology turned off. Model simulation results were compared to actual chlorophyll distributions (MODIS data) for June 5th (3 days of forecast) and June 10th (8 days of forecast). Comparisons of ensembles E1 and E2 provide the assessment of the bio-chemical model contribution to the variability and uncertainty in the chlorophyll forecasts in comparison to the case where chlorophyll is treated as the passive tracer and controlled only by advective and diffusive processes (Figure 10).

The E1 ensemble chlorophyll mean reproduced the observed productivity (chlorophyll values) inside the Bay after 3 days (June 5th), and especially after 8 days (June 10th) of simulation. Also, the E1 ensemble mean reproduced the observed increase in productivity from June 5th to June 10th. The primary modeling focus of the field program was on predictions inside the Bay (especially in the upwelling shadow area in the northern part of the Bay), and is encouraging given that the model demonstrated good skill in chlorophyll predictions even without any bio-chemical data assimilation. The E2 ensemble chlorophyll mean (reminder that the chlorophyll is treated as passive tracer in the E2) demonstrated significantly reduced productivity inside the Bay in comparison to observations during 8 days of simulations. Also, ensemble E2 did not reproduce the observed increase of productivity from June 5th to June 10th. In addition, the variability in ensemble E2 predictions is much lower in comparison to the variability in ensemble E1. These results show that in upwelling dominated areas (like along the West Coast of US); the coupling to bio-chemical model is needed to reproduce the observed chlorophyll variability along the coast even for short-term forecasts (only advective and diffusive processes are not able to reproduce observed productivity). On June 5th (3 days of simulation), the root mean square (RMS) error for ensemble E1 is 80 % less than for ensemble E2

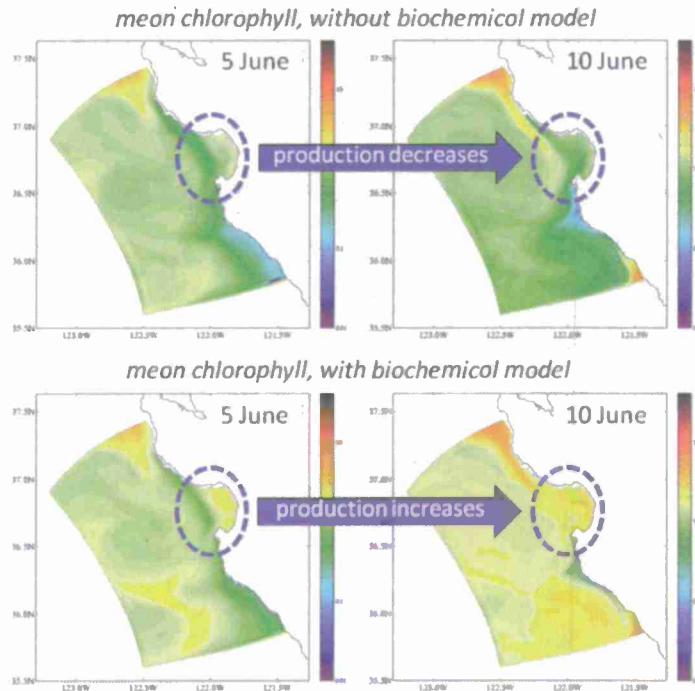


Figure 10. E1 (bottom panel, with biology) and E2 (top panel, without biochemical model) ensemble model results for Monterey Bay, June 1008. With biology included, the results more closely match the MODIS image for 10 June in the bay.

inside the Bay. For June 10th (8 days of simulations), the RMS error for ensemble E1 is 53% (almost double) less than for E2. Outside the Bay, the ensemble E1 mean demonstrated higher than observed productivity. This is due to the fact that rates of grazing, mortality, nutrients uptakes, CHL to nitrogen ratios etc are the same through the model domain while ecosystems inside and outside the Bay are quite different. Good model predictions inside the Bay indicate that the ecosystem model parameters are appropriate for dynamics inside the bay, but should be corrected outside the Bay. This is a complicated task due to lack of observations to constrain the ecosystem model parameters. Preliminary experiments with assimilating satellite ocean color data for a better initialization of the bio-chemical model constituents show improvement in the model offshore chlorophyll predictions (Shulman et al., 2012).

DISCUSSION AND SUMMARY

The environmental modeling community commonly employs an ensemble approach to propagate initialization, forcing, and algorithm error sources through the simulation process. We have extended this approach to satellite ocean color image processing/analysis, to allow quantitative error evaluations and error cascading, and to estimate uncertainties in the derived bio-optical products. In addition to analysis of the satellite chlorophyll uncertainty, we further incorporated this uncertainty into short-term (1-3 day) hydrodynamic forecasts of the chlorophyll field. We examined the effect of including biology in the forecast by coupling the hydrodynamic model to an ecosystem model. We compared the forecast distributions with actual distributions observed from satellite imagery, and employed spread-skill statistics as a metric to assess forecast errors.

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